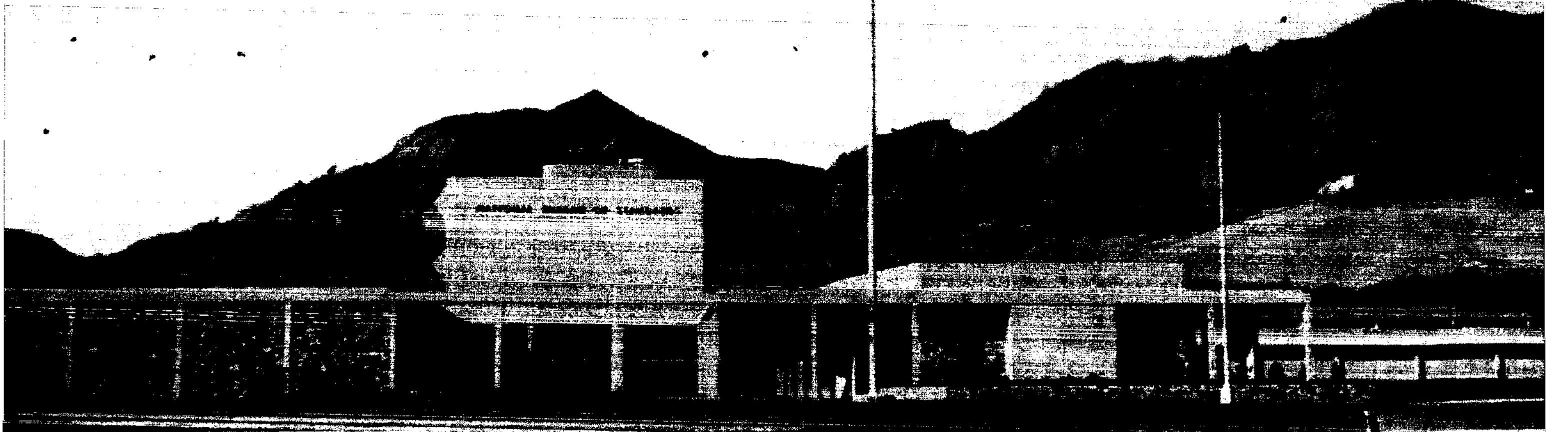

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IBM 7090 FORTRAN II PROGRAM FOR THERMODYNAMIC PROPERTY COMPUTATIONS

Enthalpy-Pressure or Pressure-Density as Independent Coordinates

UNPUBLISHED PRELIMINARY DATA

J. G. Hust

NBS

U. S. DEPARTMENT OF COMMERCE
NATIONAL BUREAU OF STANDARDS
BOULDER LABORATORIES
Boulder, Colorado

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U.S. DEPARTMENT OF COMMERCE

NATIONAL BUREAU OF STANDARDS

CONTENTS

IBM 7090 FORTRAN II PROGRAM FOR THERMODYNAMIC PROPERTY COMPUTATIONS

Enthalpy-Pressure or Pressure-Density as Independent Coordinates*

J. G. Hust

15337

Two FORTRAN II subroutines for the calculation of thermodynamic properties of oxygen using pressure and density or pressure and enthalpy as independent coordinates are described. The numerous function subprograms and subroutines required for execution of these computations are also described. Listings of all FORTRAN decks are included along with brief descriptions of the basic mathematical methods employed.

Author

1. INTRODUCTION

In a previous publication [Hust and Gosman, 1964] methods of calculating thermodynamic properties from equations of state were presented. Parallel developments with density-temperature and pressure-temperature as independent coordinates were given. In particular, an equation of state was presented together with closed form expressions for entropy, enthalpy and internal energy in terms of density and temperature as derived by Strobridge [1962]. In many instances, however, it is either desirable or necessary to calculate thermodynamic properties from other coordinates, such as pressure and temperature or pressure and density or enthalpy and pressure. It therefore becomes necessary to either invert the equations for the desired variables or to solve the given set of equations by iterative methods. Since it is frequently impossible to invert such equations in closed form, the iterative technique seems more desirable.

Computer programs have been developed to perform this inversion by iterative methods for pressure-enthalpy and pressure-density as independent coordinates. This package, as presented here, is applicable only to oxygen property calculations, and contains preliminary coefficients for the equation of state as well as a preliminary vapor pressure equation presented by Stewart, et al. [1963]. Improved coefficients

* This report is a result of a study made by the Cryogenic Data Center of the Cryogenic Engineering Laboratory under a contract with the National Aeronautics and Space Administration.

for this equation of state and a more accurate vapor pressure equation will be published in the near future, which may then be substituted in this program. This paper presents the mathematical methods used, and descriptions and listings of the FORTRAN II programs required. Sample results for oxygen with comparisons to the tabular values presented by Stewart, et al. [1963], are also given.

Coefficients for this equation of state are also available* for nitrogen, carbon monoxide, argon, and hydrogen. Therefore, with relatively simple changes, this program can be adapted for the calculation of the properties of these other fluids. The coefficients of this equation of state for these fluids may be obtained from the following references:

nitrogen - Strobridge, T. R., Natl. Bur. Standards Tech. Note No. 129, PB 161630 (1962)

carbon monoxide - Hust, J. G., and R. B. Stewart, Natl. Bur. Standards Tech. Note No. 202 (1963)

argon - Gosman, A. L., J. G. Hust, and R. D. McCarty, Natl. Bur. Standards Rept. No. 8293

hydrogen - Roder, H. M., and R. D. Goodwin, Natl. Bur. Standards Tech. Note 130, PB 161631

2. MATHEMATICAL METHODS

The general iterative methods are illustrated as follows: Consider the independent variables of a given problem to be x and y and the dependent variables u and v to be related functionally as

$$u = u(x, y) \tag{1}$$

and

$$v = v(x, y). \tag{2}$$

* Copies of these references are available from the Cryogenic Data Center, National Bureau of Standards, Boulder, Colorado.

(a) Case I - Both "dependent" variables are specified while the "independent" variables are to be determined.

One writes the differentials du and dv as

$$du = \left(\frac{\partial u}{\partial x} \right)_y dx + \left(\frac{\partial u}{\partial y} \right)_x dy \tag{3}$$

and

$$dv = \left(\frac{\partial v}{\partial x} \right)_y dx + \left(\frac{\partial v}{\partial y} \right)_x dy. \tag{4}$$

These equations are considered to be approximations if the differential quantities are replaced by finite increments. If one makes initial estimates of x_i and y_i for x and y, then (3) and (4) can be written as

$$\Delta u_i = u - u\,(x_i, y_i) \cong \left(\frac{\partial u}{\partial x} \right)_y \Delta x_i + \left(\frac{\partial u}{\partial y} \right)_x \Delta y_i \tag{5}$$

and

$$\Delta v_i = v - v\,(x_i, y_i) \cong \left(\frac{\partial v}{\partial x} \right)_y \Delta x_i + \left(\frac{\partial v}{\partial y} \right)_x \Delta y_i. \tag{6}$$

The increments Δx_i and Δy_i are evaluated from (5) and (6) and second estimates for x and y become

$$x_{i+1} = x_i + \Delta x_i \tag{7}$$

and

$$y_{i+1} = y_i + \Delta y_i. \tag{8}$$

The process is then repeated until the absolute values of Δu_i and Δv_i or Δx_i and Δy_i are less than some predetermined values. Convergence depends upon the behavior of the function and the initial estimates for x and y. This method is described in more detail by Nielsen [1956]. Considering the Strobridge equation for pressure in terms of density and temperature and the resulting enthalpy equation, we observe that the calculation of density and temperature from enthalpy and pressure may be accomplished by this method. The derivatives required

to perform this iteration are $(\partial H/\partial T)_D$, $(\partial H/\partial D)_T$, $(\partial P/\partial T)_D$, and $(\partial P/\partial D)_T$, where H is enthalpy, P is pressure, T is temperature, and D is density.

(b) Case 2 - Both a "dependent" and an "independent" variable are specified.

When a dependent and an independent variable are specified, such as u and x, the calculation is performed with the more commonly used Newton-Raphson iteration in one dimension. One first inverts, by iteration, the function $u = u(x, y)$ for the value of y. Then v is calculated directly.

The calculation of enthalpy and temperature from pressure and density using the Strobridge equation is of this type. The derivative required to perform the Newton-Raphson iteration for temperature is $(\partial P/\partial T)_D$.

3. PROGRAM DESCRIPTION

The general description of each subprogram is presented to clarify its purpose in the overall program. A listing of each FORTRAN deck is also included to present the details of each computation.

Subroutine TDSTRS (13 arguments) calculates temperature, density, and entropy (and quality in the two-phase region) for given values of pressure and enthalpy. Subroutine THSTRS (12 arguments) calculates temperature, enthalpy, and entropy (and quality in the two-phase region) for given values of pressure and density. Both of these subroutines also contain two fixed point arguments; one of which indicates the region (i.e., gaseous, liquid, or two-phase) dictated by the input pressure and enthalpy or pressure and density, and the other indicates discrepancies encountered either in the input data or the execution of the program. These arguments may be printed in the output (see example in Appendix B).

The above subroutines call the following subroutine and function subprograms. The purpose of the quantities calculated by these functions can be more readily recognized by referring to equations (28) through (43) in the paper by Hust and Gosman [1964].

Functions PSFITZ(T,D,AEXP,A15,IUSE), DPDDRS(T,D,AEXP,A15,IUSE), and DPDTTS(T,D,AEXP,A15,IUSE) calculate pressure, $(\partial P/\partial D)_T$, and $(\partial P/\partial T)_D$ according to the Strobridge equation, respectively. The arguments have the following meaning: D is density, T is temperature, AEXP is the coefficient in the exponential term, A15 is the 15 element array containing the coefficients other than the gas constant and AEXP. It should be noted that the ordering of the terms in these functions is not the same as that indicated by Strobridge. The manipulation of the 17 element array of coefficients to obtain the 15 element array is accomplished by subroutine ARCOE(A17,A15). The remaining argument IUSE designates whether the functions calculate the above quantities or if they are being used in setting up a least squares matrix. The reason for the re-ordering of the terms and the details of the dual nature of these programs would not contribute to this discussion, and so are not presented here.

Function FINDPS(T,P,DTRI,AEXP,A15) iterates, by the Newton-Raphson method, to obtain the density for a given pressure and temperature as related by the Strobridge equation. If the Newton-Raphson method fails to converge, the method of regula falsi is also tried (Hildebrand [1956]). An error statement is written on the systems output tape if either of these iterations fails to converge. The arguments have the same meaning as the previous functions with the addition of DTRI which is the first trial density and P which is pressure. Function FINTPS(D,P,TTRI,AEXP,A15) is the same as FINDPS with the exception that temperature is the unknown. TTRI is the first trial in temperature.

Functions VPN(T) and DPDTVP(T) compute the vapor pressure and its derivative with respect to temperature, respectively. Function FINDT(P,TLO,TUP) calculates the saturation temperature for a given vapor

pressure. TLO and TUP must be less than, and greater than the saturation temperature, respectively. For example, TLO and TUP may be taken as the triple point and critical point temperatures, respectively.

Functions DELS1S(D,T,A17) and DELH1S(P,D,T,A17) along with functions CPOSJ(T,TO) and CPOHJ(T,TO) are used to calculate entropy and enthalpy in the gaseous region. Function CPOHJ(T,TO) represents the integral of the specific heat at zero pressure from the reference temperature, TO, to the temperature T; while DCPOHJ(T) represents the zero pressure specific heat at temperature T. Function CPOSJ(T,TO) is used to calculate the integral of C_p^o/T with respect to temperature from TO to T.

Functions DELSTS(D2,D1,T,A17) and DELHTS(P2,D2,P1,D1,T,A17) calculate the isothermal changes in entropy and enthalpy from the point P1,D1,T to the point P2,D2,T. These functions are used in the liquid range but are valid for the gaseous range as well except at zero density. The derivative $(\partial H/\partial T)_D$ for the gaseous range is determined by function DHDTRS(D,T,A17). The same derivative in the liquid region is obtained from finite differences within subroutine TDSTRS (13 arguments). The derivative $(\partial H/\partial D)_T$ is obtained with function DHDDRS(D,T,A17).

4. REFERENCES

Hildebrand, F. B. (1956), Introduction to Numerical Analysis (McGraw-Hill Book Company, Inc., New York).

Hust, J. G., and A. L. Gosman (1964), Functions for the Calculation of Entropy, Enthalpy, and Internal Energy for Real Fluids Using Equations of State and Specific Heats, Advances in Cryogenic Engineering 9, 227-33 (Plenum Press, New York).

Nielsen, K. L. (1956), Methods in Numerical Analysis (The Mac Millan Company, New York).

Stewart, R. B., J. G. Hust, and R. D. McCarty (1963), Interim Thermodynamic Properties for Gaseous and Liquid Oxygen at Temperatures from 55 to 300°K and Pressures to 300 Atmospheres, Natl. Bur. Standards Rept. No. 7922.

Strobridge, T. R. (1962), The Thermodynamic Properties of Nitrogen from 64 to 300°K between 0.1 and 200 Atmospheres, Natl. Bur. Standards Tech. Note No. 129, PB 161630.

APPENDIX A

The following is an alphabetical listing of all FORTRAN subprograms required to obtain thermodynamic properties with pressure and enthalpy or pressure and density as input coordinates. The calling sequence is illustrated in APPENDIX B. Punched card decks of these fortran II subprograms may be obtained from the Cryogenic Data Center, National Bureau of Standards, Boulder, Colorado.

Contents

* These subprograms are restricted to oxygen property calculation.

‡ The vapor pressure equation used here is in preliminary form, according to Stewart, et al. [1963]. An improved relation will be published in the near future.

† The coefficients used here in the equation of state are preliminary, according to Stewart, et al. [1963]. Improved values will be published in the near future.

```
      SUBROUTINE ARCOE(ATRS,APS)
C     REORDERING OF THE COEFFICIENTS FOR THE STROBRIDGE EQUATION OF
C     STATE AS USED IN PSFITZ,DPDDRS, AND DPDTTS. THE INPUT MATRIX IS
C     ATRS(17) AND THE OUTPUT MATRIX IS APS(15).
      DIMENSION ATRS(17),APS(15)
      APS(1)=ATRS(16)
      APS(2)=ATRS(9)
      APS(3)=ATRS(7)
      APS(4)=ATRS(8)
      APS(5)=ATRS(2)
      APS(6)=ATRS(3)
      APS(7)=ATRS(4)
      APS(8)=ATRS(13)
      APS(9)=ATRS(10)
      APS(10)=ATRS(14)
      APS(11)=ATRS(5)
      APS(12)=ATRS(15)
      APS(13)=ATRS(11)
      APS(14)=ATRS(6)
      APS(15)=ATRS(12)
      RETURN
      END


      FUNCTION CPOHJ(T,TO)
C     INTEGRAL OF ZERO PRESSURE SPECIFIC HEAT FROM TO TO T WITH RESPECT
C     TO TEMPERATURE. TEMPERATURE IN DEG K AND CPOHJ IN JOULES/MOLE.
      R=0.0620997 *4.184*32.0
      G1=3.5043099
      G2=-0.68438341E-04
      G3=0.81799927E-06
      G4=-0.58262431E-08
      G5=0.16619840E-10
      TD1=T-TO
      TD2=(T**2-TO**2)/2.0
      TD3=(T**3-TO**3)/3.0
      TD4=(T**4-TO**4)/4.0
      TD5=(T**5-TO**5)/5.0
      CPOH=(G1*TD1+G2*TD2+G3*TD3+G4*TD4+G5*TD5)*R
      CPOHJ=CPOH
      RETURN
      END


      FUNCTION CPOSJ(T,TO)
C     INTEGRAL OF ZERO PRESSURE SPECIFIC HEAT DIVIDED BY TEMPERATURE
C     FROM TO TO T WITH RESPECT TO TEMPERATURE. TEMPERATURE IN DEG K AND
```

```
C     CPOSJ IN JOULES/(MOLE DEG K).
      R=0.0620997*4.184*32.0
      G1=3.5043099
      G2=-0.68438341E-04
      G3=0.81799927E-06
      G4=-0.58262431E-08
      G5=0.16619840E-10
      TD1=T-TO
      TD2=(T**2-TO**2)/2.0
      TD3=(T**3-TO**3)/3.0
      TD4=(T**4-TO**4)/4.0
      CPOS=(G1*LOGF(T/TO)+G2*TD1+G3*TD2+G4*TD3+G5*TD4)*R
      CPOSJ=CPOS
      RETURN
      END


      FUNCTION DCPOHJ(TEMP)
C     ZERO PRESSURE SPECIFIC HEAT IN JOULES/MLE. TEMPERATURE IN DEG K.
      R=8.3144
      T=TEMP
      G1=3.5043099
      G2=-0.68438341E-04
      G3=0.81799927E-06
      G4=-0.58262431E-08
      G5=0.16619840E-10
      DCPOH=(G1+G2*T+G3*T**2+G4*T**3+G5*T**4)*R
      DCPOHJ=DCPOH
      RETURN
       END


      FUNCTION DELHTS(P2,D2,P1,D1,T,A)
C     ISOTHERMAL CHANGE OF ENTHALPY FROM THE STATE D1,P1,T TO THE STATE
C     D2,P2,T USING THE STROBRIDGE EQUATION OF STATE. D1 AND D2 MUST BE
C     GREATER THAN ZERO. PRESSURE IN ATM, DENSITY IN MOLES/LITER, TEMP-
C     ERATURE IN DEG K, AND DELHTS IN JOULES/MOLE.
      DIMENSION A(17)
      P=P1
      D=D1
     0ENTHA1=P/D+D*(A(3)+2.0*A(4)/T+3.0*A(5)/T**2+5.0*A(6)/T**4)+A(8)*D
     1     *D/2.0-(3.0*A(10)/T**2+4.0*A(11)/T**3+5.0*A(12)/T**4)*EXPF
     2     (-A(17)*D*D)/(2.0*A(17))-(D*D/(2.0*A(17))+1.0/(2.0*A(17)**2))
     3     *(3.0*A(13)/T**2+4.0*A(14)/T**3+5.0*A(15)/T**4)*
     4      EXPF(-A(17)*D*D)+A(16)*D**5/5.0
      P=P2
      D=D2
     0ENTHA2=P/D+D*(A(3)+2.0*A(4)/T+3.0*A(5)/T**2+5.0*A(6)/T**4)+A(8)*D
     1     *D/2.0-(3.0*A(10)/T**2+4.0*A(11)/T**3+5.0*A(12)/T**4)*EXPF
     2     (-A(17)*D*D)/(2.0*A(17))-(D*D/(2.0*A(17))+1.0/(2.0*A(17)**2))
     3     *(3.0*A(13)/T**2+4.0*A(14)/T**3+5.0*A(15)/T**4)*
     4      EXPF(-A(17)*D*D)+A(16)*D**5/5.0
```

```
      DELHTS=(ENTHA2-ENTHA1)*101.3278
      RETURN
      END


      FUNCTION DELH1S(P2,D2,T,A )
C     ISOTHERMAL CHANGE IN ENTHALPY FROM ZERO DENSITY TO THE POINT P2,D2
C     ,T USING THE STROBRIDGE EQUATION OF STATE.
C     PRESSURE IN ATM, TEMPERATURE IN DEG K, DENSITY IN MOLES/LITER, AND
C     DELH1S IN JOULES/MOLE.
      DIMENSION A(17)
      P=P2
      D=D2
      EX=EXPF(-A(17)*D*D)
     0DELH1S=(P/D-A(1)*T+D*(A(3)+2.0*A(4)/T+3.0*A(5)/T**2 +5.0*A(6)/T**4
     1    )+A(8)*D*D/2.0 -(3.0*A(10)/T**2 +4.0*A(11)/T**3+5.0*A(12)/
     2    T**4)*EX/(2.0*A(17))-(D**2/(2.0*A(17))+1.0/(2.0*A(17)**2))
     3    *(3.0*A(13)/T**2+4.0*A(14)/T**3+5.0*A(15)/T**4)*EX
     4    +A(16)*D**5/5.0+(3.0*A(10)/T**2+4.0*A(11)/T**3+5.0*A(12)
     5     /T**4)/(2.0*A(17))+(3.*A(13)/T**2+4.0*A(14)/T**3+
     6    5.0*A(15)/T**4)/(2.0*A(17)**2))*101.3278
      RETURN
      END


      FUNCTION DELSTS(D2,D1,T,A)
      DIMENSION A(17)
C     ISOTHERMAL CHANGE IN ENTROPY FROM THE STATE SPECIFIED BY D1,T TO
C     THE STATE SPECIFIED BY D2,T USING THE STROBRIDGE EQUATION OF STATE
C     . D2 AND D1 MUST BE GREATER THAN ZERO. PRESSURE IN ATM, TEMPERA-
C     TURE IN DEG K, AND DELSTS IN JOULES/(MOLE DEG K).
      D=D2
     0ENTRO2=(-D*(A(2)*A(1)-A(4)/T**2-2.0*A(5)/T**3-4.0*A(6)/T**5)
     1     -A(7)*A(1)*D**2/2.0-A(9)*D**3/3.0-(2.0*A(10)/T**3+3.0*A(11)/
     2     T**4+4.0*A(12)/T**5)*EXPF(-A(17)*D*D)/(2.0*A(17))
     3     -(D*D/(2.0*A(17))+1.0/(2.0*A(17)**2))*(2.0*A(13)/T**3
     4     +3.0*A(14)/T**4+4.0*A(15)/T**5)*EXPF(-A(17)*D*D)-A(1)*LOGF(D)
     5     )*101.3278
      D=D1
     0ENTRO1=(-D*(A(2)*A(1)-A(4)/T**2-2.0*A(5)/T**3-4.0*A(6)/T**5)
     1     -A(7)*A(1)*D**2/2.0-A(9)*D**3/3.0-(2.0*A(10)/T**3+3.0*A(11)/
     2     T**4+4.0*A(12)/T**5)*EXPF(-A(17)*D*D)/(2.0*A(17))
     3     -(D*D/(2.0*A(17))+1.0/(2.0*A(17)**2))*(2.0*A(13)/T**3
     4     +3.0*A(14)/T**4+4.0*A(15)/T**5)*EXPF(-A(17)*D*D)-A(1)*LOGF(D)
     5     )*101.3278
      DELSTS=ENTRO2-ENTRO1
      RETURN
      END


      FUNCTION DELS1S(D2,T,A)
```

```
C     ISOTHERMAL CHANGE IN ENTROPY FROM THE IDEAL GAS STATE AT 1 ATM AND
C     T DEG K TO THE STATE SPECIFIED BY D2,T ON THE REAL GAS SURFACE.
C     TEMPERATURE IN DEG K, DENSITY IN MOLES/LITER, AND DELS1S IN JOULES
C     /(MOLE DEG K).
      DIMENSION A(17)
      D=D2
      EX=EXPF(-A(17)*D*D)
     0DELS1S=(-A(1)*LOGF(A(1)*T*D)-D*(A(2)*A(1)-A(4)/T**2-2.0*A(5)/T**3-
     1     4.0*A(6)/T**5)-A(7)*A(1)*D*D/2.0-A(9)*D**3/3.0-
     2     EX*(2.0*A(10)/T**3+3.0*A(11)/T**4+4.0*A(12)/T**5)/
     3     (2.0*A(17))-(D*D/(2.0*A(17))+1.0/(2.0*A(17)**2))*
     4     (2.0*A(13)/T**3+3.0*A(14)/T**4+4.0*A(15)/T**5)*EX+
     5     (2.0*A(10)/T**3+3.0*A(11)/T**4+4.0*A(12)/T**5)/(2.0*A(17))+
     6     (2.0*A(13)/T**3+3.0*A(14)/T**4+4.0*A(15)/T**5)/
     7     (2.0*A(17)**2))*101.3278
      RETURN
      END


      FUNCTION DHDDRS(DENS,TEMP,A)
C     DERIVATIVE OF ENTHALPY WITH RESPECT TO DENSITY AT CONSTANT TEMPER-
C     ATURE WITH THE STROBRIDGE EQUATION OF STATE.(VALID FOR VAPOR AND
C     LIQUID) DENSITY IN MOLES/LITER, TEMPERATURE IN DEG K, AND DHDDRS
C     IN JOULES LITER/(MOLE MOLE).
      DIMENSION A(17),AA(15)
      D =DENS
      T=TEMP
      A16=A(17)
      CALL ARCOE(A,AA)
      DHDDRS=-T*DPDTTS(T,D,A16,AA,0)/(D*D)+DPDDRS(T,D,A16,AA,0)/D
      DHDDRS=DHDDRS*101.3278
      RETURN
      END


      FUNCTION DHDTRS(DEN,TEMP,A)
C     DERIVATIVE OF ENTHALPY WITH RESPECT TO TEMPERATURE AT CONSTANT
C     DENSITY WITH THE STROBRIDGE EQUATION OF STATE. (VALID FOR VAPOR
C     ONLY) DENSITY IN MOLES/LITER, TEMPERATURE IN DEG K, AND DHDTRS IN
C     JOULES/(MOLE DEG K).
      DIMENSION A(17)
      CON=101.3278
      D=DEN
      D2=D*D
      D3=D*D2
      D4=D*D3
      D5=D*D4
      T=TEMP
      T2=T*T
      T3=T*T2
      T4=T*T3
      T5=T*T4
```

```
      EX=EXPF(D2*(-A(17)) )
      DHD1=A(1)+D*(A(1)*A(2)-A(4)/T2-2.*A(5)/T3-4.*A(6)/T5)+D2*A(7)*A(1)
     1+D3*A(9)-D2*(2.0*A(10)/T3+3.0*A(11)/T4+4.0*A(12)/T5)*EX
     2-D4*(2.0*A(13)/T3+3.0*A(14)/T4+4.0*A(15)/T5)*EX
     3-A(1)-D*(2.0*A(4)/T2+6.0*A(5)/T3+20.0*A(6)/T5)+EX*(6.0*A(10)/T3+
     412.0*A(11)/T4+20.0*A(12)/T5)/(2.0*A(17))+(D2/(2.0*A(17))+1.0/(2.0*
     5A(17)**2))*EX*(6.0*A(13)/T3+12.0*A(14)/T4+20.0*A(15)/T5)-(6.0*
     6A(10)/T3+12.0*A(11)/T4+20.0*A(12)/T5)/(2.0*A(17))-(6.0*A(13)/T3+
     712.0*A(14)/T4+20.0*A(15)/T5)/(2.0*A(17)**2)
      DHD1=DHD1*CON
      DHDTRS=DHD1+DCPOHJ(T)
      RETURN
      END


      FUNCTION DPDDRS(T,D,A16,A,IUSE)
C     IF IUSE =0
C     CALCULATE DERIVATIVE OF PRESSURE WITH RESPECT TO DENSITY AT
C     CONSTANT TEMPERATURE WITH THE STROBRIDGE EQUATION OF STATE.
C     A(15) IS THE LINEAR COEFFICIENT MATRIX WHILE A16 IS THE EXPONENT.
C     IF IUSE =1
C     CALCULATE THE VARIABLE PART OF EACH TERM AND RETURN TO THE MAIN
C     PROGRAM THRU A(15) FOR USE IN SETTING UP LEAST SQUARES PROBLEM.
C     DENSITY IN MOLES/LITER, TEMPERATURE IN DEG K, AND DPDDRS IN ATM
C     LITERS/(MOLE MOLE).
      DIMENSION A(15),B(15)
      D2=D*D
      D3=D2*D
      D4=D3*D
      D5=D4*D
      D6=D5*D
      T2=T*T
      T3=T2*T
      T4=T3*T
      EX=EXPF(-A16*D2)
      R=0.0820797
      B(1)=6.0*D5
      B(2)=4.0*T*D3
      B(3)=3.0*R*T*D2
      B(4)=3.0*D2
      B(5)=2.0*R*T*D
      B(6)=2.0*D
      B(7)=2.0*D/T
      B(8)=(5.0*D4-2.0*A16*D6)*EX/T2
      B(9)=(3.0*D2-2.0*A16*D4)*EX/T2
      B(10)=B(8)/T
      B(11)=2.0*D/T2
      B(12)=B(8)/T2
      B(13)=B(9)/T
      B(14)=2.0*D/T4
      B(15)=B(9)/T2
      DPDDRS=R*T
      IF(IUSE)10,20,10
```

```
   10 DO 12 I=1,15
   12 A(I)=B(I)
      DPDDRS=-DPDDRS
      RETURN
   20 DO 30 I=1,15
   30 DPDDRS=DPDDRS+A(I)*B(I)
      RETURN
      END


      FUNCTION DPDTTS(T,D,A16,A,IUSE)
C     IF IUSE =0
C     CALCULATE DERIVATIVE OF PRESSURE WITH RESPECT TO TEMPERATURE AT
C     CONSTANT DENSITY WITH THE STROBRIDGE EQUATION OF STATE.
C     A(15) IS THE LINEAR COEFFICIENT MATRIX WHILE A16 IS THE EXPONENT.
C     IF IUSE =1
C     CALCULATE THE VARIABLE PART OF EACH TERM AND RETURN TO THE MAIN
C     PROGRAM THRU A(15) FOR USE IN SETTING UP LEAST SQUARES PROBLEM.
C     DENSITY IN MOLES/LITER, TEMPERATURE IN DEG K, AND DPDTTS IN ATM/
C     DEG K.
      DIMENSION A(15),B(15)
      D2=D*D
      D3=D2*D
      D4=D3*D
      D5=D4*D
      D6=D5*D
      D7=D6*D
      T2=T*T
      T3=T2*T
      T4=T3*T
      T5=T4*T
      EX=EXPF(-A16*D2)
      R=0.0820797
      B(1)=0.0
      B(2)=D4
      B(3)=R*D3
      B(4)=0.0
      B(5)=R*D2
      B(6)=0.0
      B(7)=-D2/T2
      B(8)=-2.0*D5*EX/T3
      B(9)=-2.0*D3*EX/T3
      B(10)=-3.0*D5*EX/T4
      B(11)=-2.0*D2/T3
      B(12)=-4.0*D5*EX/T5
      B(13)=-3.0*D3*EX/T4
      B(14)=-4.0*D2/T5
      B(15)=-4.0*D3*EX/T5
      DPDTTS=D*R
      IF(IUSE)10,20,10
   10 DO 12 I=1,15
   12 A(I)=B(I)
      DPDTTS=-DPDTTS
```

```
      RETURN
   20 DO 30 I=1,15
   30 DPDTTS=DPDTTS+A(I)*B(I)
      RETURN
      END


      FUNCTION DPDTVP(TEMP)
C     DERIVATIVE OF VAPOR PRESSURE WITH RESPECT TO TEMPERATURE AS IN
C     NBS REPORT 7922. TEMPERATURE IN DEG K AND DPDTVP IN ATM/DEG K.
      PC=50.14
      TC=154.78
      T=TEMP
      A=0.13750055E-03
      B=-0.54998814E-01
      C=0.17023470E+01
      D=0.66564191E+01
      E=-0.94512173E+03
      P=EXPF(D+E/T+B*T+C*LOGF(T)+A*T*T)
      DPVPO2=TC/PC*P*(2.*A*T+B+C/T-E/(T*T))
      DPDTVP=DPVPO2*PC/TC
      RETURN
      END


      FUNCTION DSATLI(TEMP)
C     DENSITY OF SATURATED LIQUID OXYGEN ACCORDING TO SCOTT. TEMPERATURE
C     IN DEG K AND DSATLI IN MOLES/LITER.
      T=TEMP
      DSCOTR=1.0+(154.78-T)**0.4/((7.106+0.0038*T)*.43)
      DSATLI=DSCOTR*1000.028*0.43/32.0
      RETURN
      END


      FUNCTION DSVGUR(TR)
C     REDUCED DENSITY OF SATURATED VAPOR AT REDUCED TEMPERATURE TR.
C     DISCONTINUOUS AT TR=0.65. APPROXIMATION PRESENTED BY GUGGENHEIM.
    1 IF(TR-0.65)3,2,2
    2 DSVGUR=1.0+0.75*(1.0-TR)-(7.0/4.0)*(1.0-TR)**(1.0/3.0)
      RETURN
    3 PR=EXPF(5.29-5.31/TR)
      ZC=0.3
      DSVGUR=PR*ZC/TR
      RETURN
      END


      FUNCTION FINDPS(TT,PP,DDTRI,SSUD,A)
C     CALCULATE DENSITY AT A GIVEN PRESSURE AND TEMPERATURE FROM THE
```

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C     STROBRIDGE EQUATION OF STATE BY THE NEWTON-RAPHSON METHOD USING
C     PSFITZ AND DPDDRS. IF THE ITERATION FAILS TO CONVERGE, THE METHOD
C     OF REGULA FALSI IS ALSO TRIED. IF EITHER METHOD FAILS AN ERROR
C     STATEMENT IS WRITTEN ON THE SYSTEM OUTPUT TAPE.
      DIMENSION A(15)
      T=TT
      P=PP
      DTRI=DDTRI
      SUD=SSUD
      DSTART=DTRI
      DO 20 I=1,10
      Z=PSFITZ(T,DTRI,SUD,A,0)-P
      ZZ=DPDDRS(T,DTRI,SUD,A,0)
      DTRI=DTRI-Z/ZZ
      IF(ABSF(Z/P)-0.000001)30,30,10
   10 IF(ABSF(Z/(ZZ*DTRI))-0.000001)30,30,20
   20 CONTINUE
      WRITE OUTPUT TAPE 6,100,T,P,DSTART,DTRI
C     THIS COMPLETES THE NEWTON-RAPHSON  ITERATION PROCEDURE
      GO TO 40
   30 FINDPS=DTRI
      RETURN
   40 DUP=DSTART
      DDWN=DSTART
 1000FORMAT(88HNEWTON-RAPHSON  METHOD FAILED TO PRODUCE SIX SIGNIFICANT
     1FIGURE ACCURACY IN 10 ITERATIONS/62H    TEMPERATURE      PRESSURE
     2    FIRST DENSITY    TENTH DENSITY/ 4E16.8)
      DELD=1.01
      DO 50 I=1,200
      DUP=DUP*DELD
      DDWN=DDWN/DELD
      ZUP=PSFITZ(T,DUP,SUD,A,0)-P
      ZDWN=PSFITZ(T,DDWN,SUD,A,0)-P
      RATIO=ZUP/ZDWN
      IF(RATIO)60,110,50
   50 CONTINUE
      WRITE OUTPUT TAPE 6,200,DSTART,T,P,DDWN,DUP
  200 FORMAT(77HNO SOLUTION HAS BEEN FOUND BETWEEN 1.0/7.4 AND 7.4 OF TH
     1E INITIAL DENSITY    =,E18.8,/64H    TEMPERATURE      PRESSURE
     2LOWER DENSITY    UPPER DENSITY /4E16.8)
      FIND PS=0.0
      RETURN
   60 ZUP1=PSFITZ(T,DUP/DELD,SUD,A,0)-P
      UPRAT=ZUP /ZUP1
      IF(UPRAT)80,110,70
   70 D2=DDWN*DELD
      D1=DDWN
      GO TO 90
   80 D2=DUP
      D1=DUP/DELD
   90 DO 95 I=1,100
      Z1=PSFITZ(T,D1,SUD,A,0)-P
      Z2=PSFITZ(T,D2,SUD,A,0)-P
      D3=D1+(D2-D1)*(-Z1)/(Z2-Z1)
```

```
      IF(ABSF((D1-D2)/D1)-0.000001)99,99,91
   91 IF(ABSF((Z1-Z2)/(Z1+P))-0.000001)99,99,92
   92 Z3=PSFITZ(T,D3,SUD,A,0)-P
      IF(Z3/Z1)93,99,94
   93 Z2=Z3
      D2=D3
      GO TO 95
   94 Z1=Z3
      D1=D3
   95 CONTINUE
      WRITE OUTPUT TAPE 6,300,T,P,D1,D2
  3000FORMAT(87HREGULA-FALSI METHOD FAILED TO PRODUCE SIX S+GNIFICANT FI
     1GURE ACCURACY IN 100 ITERATIONS/64H    TEMPERATURE     PRESSURE
     2    LOWER DENSITY    UPPER DENSITY /4E16.8)
   99 FINDPS=D3
      RETURN
  110 FINDPS=DUP
      RETURN
      END


      FUNCTION FINDT(PRESS,TLO,TUP)
C     NEWTON-RAPHSON ITERATION TO FIND THE SATURATION TEMPERATURE CORR-
C     ESPONDING TO THE PRESSURE. TLO AND TUP ARE THE INDICATED LOWER
C     AND UPPER TEMPERATURE BOUNDS WITHIN WHICH THE RESULT MUST LIE.
C     THESE TEMPERATURES ARE ALSO USED IN DETERMINING THE FIRST TRIAL.
C     THE FIRST TRIAL IS FOUND BY LINEAR INTERPOLATION OF LOG(P)=A+B/T.
      P=PRESS
      T2=TUP
      T1=TLO
      P2=VPN(T2)
      P1=VPN(T1)
      IF(P-P2)10,10,20
   10 IF(P-P1)35,26,26
   20 WRITE OUTPUT TAPE 6,200,P,P2
  200 FORMAT(12H1PRESSURE = ,E16.8,42H  IS GREATER THAN INDICATED UPPER
     1BOUND = ,E16.8)
      T=0.0
      RETURN
  300 FORMAT(12H1PRESSURE = ,E16.8,42H  IS  LESS THAN INDICATED LOWER BO
     1UND    = ,E16.8)
   35 WRITE OUTPUT TAPE 6,300,P,P1
      T=0.0
      RETURN
   26 CONTINUE
      B=LOGF(P2/P1)/(1.0/T2-1.0/T1)
      A=LOGF(P2)-B/T2
      TTRI=B/(LOGF(P)-A)
   31 DO 33 I=1,20
      PCAL =VPN(TTRI)
      Z=PCAL-P
      ZZ=DPDTVP(TTRI)
      DT=-Z/ZZ
```

```
      TTRI=TTRI+DT
      DPP=Z/P
      DTOT=DT/TTRI
      IF(ABSF(DPP)-0.000001)42,42,32
   32 IF(ABSF(DTOT)-0.000001)42,42,33
   33 CONTINUE
      WRITE OUTPUT TAPE 6,100,P,TTRI,PCAL
  100 FORMAT(59HNEWTON-RAPHSON ITERATION FOR TEMPERATURE FAILED TO CONVE
     1RGE/ 11HPRESSURE = ,E16.8,25HCALCULATED TEMPERATURE = ,E16.8,
     222HCALCULATED PRESSURE = ,E16.8)
   42 FINDT=TTRI
      RETURN
      END


      FUNCTION FINTPS(DD,PP,TTTRI,A16,A)
C     CALCULATE TEMPERATURE AT A GIVEN DENSITY AND PRESSURE FROM THE
C     STROBRIDGE EQUATION OF STATE BY THE NEWTON-RAPHSON METHOD USING
C     PSFITZ AND DPDDRS. IF THE ITERATION FAILS TO CONVERGE, THE METHOD
C     OF REGULA FALSI IS ALSO TRIED. IF EITHER METHOD FAILS AN ERROR
C     STATEMENT IS WRITTEN ON THE SYSTEM OUTPUT TAPE.
      DIMENSION A(15)
      D=DD
      P=PP
      TTRI=TTTRI
      SUD=A16
      TSTART=TTRI
      DO 20 I=1,10
      Z=PSFITZ(TTRI,D,SUD,A,0)-P
      ZZ=DPDTTS(TTRI,D,SUD,A,0)
      TTRI=TTRI-Z/ZZ
      IF(ABSF(Z/P)-0.000001)30,30,10
   10 IF(ABSF(Z/(ZZ*TTRI))-0.000001)30,30,20
   20 CONTINUE
      WRITE OUTPUT TAPE 6,100,D,P,TSTART,TTRI
C     THIS COMPLETES THE NEWTON-RAPHSON  ITERATION PROCEDURE
      GO TO 40
   30 FINTPS=TTRI
      RETURN
   40 TUP=TSTART
      TDWN=TSTART
 1000FORMAT(88HNEWTON-RAPHSON  METHOD FAILED TO PRODUCE SIX SIGNIFICANT
     1FIGURE ACCURACY IN 10 ITERATIONS/62H   DENSITY          PRESSURE
     2   FIRST TEMP       TENTH TEMP    / 4E16.8)
      DELT=1.01
      DO 50 I=1,100
      TUP=TUP*DELT
      TDWN=TDWN/DELT
      ZUP=PSFITZ(TUP,D,SUD,A,0)-P
      ZDWN=PSFITZ(TDWN,D,SUD,A,0)-P
      RATIO=ZUP/ZDWN
      IF(RATIO)60,110,50
   50 CONTINUE
```

```
      WRITE OUTPUT TAPE 6,200,TSTART,D,P,TDWN,TUP
  200 FORMAT(77HNO SOLUTION HAS BEEN FOUND BETWEEN 1.0/7.4 AND 7.4 OF TH
     1E INITIAL TEMP      =,E18.8,/64H   DENSITY         PRESSURE
     2LOWER TEMP      UPPER TEMP    /4E16.8)
      FINTPS=0.0
      RETURN
   60 ZUP1=PSFITZ(TUP/DELT,D,SUD,A,0)-P
      UPRAT=ZUP /ZUP1
      IF(UPRAT)80,110,70
   70 T2=TDWN*DELT
      T1=TDWN
      GO TO 90
   80 T2=TUP
      T1=TUP/DELT
   90 DO 95 I=1,100
      Z1=PSFITZ(T1,D,SUD,A,0)-P
      Z2=PSFITZ(T2,D,SUD,A,0)-P
      T3=T1+(T2-T1)*(-Z1)/(Z2-Z1)
      IF(ABSF((T1-T2)/T1)-0.000001)99,99,91
   91 IF(ABSF((Z1-Z2)/(Z1+P))-0.000001)99,99,92
   92 Z3=PSFITZ(T3,D,SUD,A,0)-P
      IF(Z3/Z1)93,99,94
   93 Z2=Z3
      T2=T3
      GO TO 95
   94 Z1=Z3
      T1=T3
   95 CONTINUE
      WRITE OUTPUT TAPE 6,300,D,P,T1,T2
  3000FORMAT(87HREGULA-FALSI METHOD FAILED TO PRODUCE SIX SIGNIFICANT FI
     1GURE ACCURACY IN 100 ITERATIONS/64H   DENSITY          PRESSURE
     2   LOWER TEMP      UPPER TEMP    /4E16.8)
   99 FINTPS=T3
      RETURN
  110 FINTPS=TUP
      RETURN
      END


      SUBROUTINE LIQCOR(S,H,TEMP)
C     ENTROPY AND ENTHALPY CORRECTIONS TO LIQUID OXYGEN BETWEEN 140 AND
C     154.77 DEG K.
C     S IN JOULES/(MOLE DEG K) AND H IN JOULES/MOLE.
      IF(TEMP-140.0)90,90,10
   10 IF(TEMP-154.77)20,90,90
   20 DELS=(0.000517857*TEMP-0.0725)*32.0
      DELH=DELS*TEMP
      S=S-DELS
      H=H-DELH
   90 RETURN
      END
```

```
      FUNCTION PSFITZ(T,D,A16,A,IUSE)
C     IF IUSE =0
C     CALCULATE PRESSURE WITH THE STROBRIDGE EQUATION OF STATE.
C     A(15) IS THE LINEAR COEFFICIENT MATRIX WHILE A16 IS THE EXPONENT.
C     IF IUSE =1
C     CALCULATE THE VARIABLE PART OF EACH TERM AND RETURN TO THE MAIN
C     PROGRAM THRU A(15) FOR USE IN SETTING UP LEAST SQUARES PROBLEM.
C     DENSITY IN MOLES/LITER, TEMPERATURE IN DEG K, AND PSFITZ IN ATM.
      DIMENSION A(15),B(15)
      D2=D*D
      D3=D2*D
      D4=D3*D
      D5=D4*D
      D6=D5*D
      T2=T*T
      T3=T2*T
      T4=T3*T
      EX=EXPF(-A16*D2)
      R=0.0820797
      B(1)=D6
      B(2)=T*D4
      B(3)=R*T*D3
      B(4)=D3
      B(5)=R*T*D2
      B(6)=D2
      B(7)=D2/T
      B(8)=D5*EX/T2
      B(9)=D3*EX/T2
      B(10)=D5*EX/T3
      B(11)=D2/T2
      B(12)=D5*EX/T4
      B(13)=D3*EX/T3
      B(14)=D2/T4
      B(15)=D3*EX/T4
      PSFITZ=D*R*T
      IF(IUSE)10,20,10
   10 DO 12 I=1,15
   12 A(I)=B(I)
      PSFITZ=-PSFITZ
      RETURN
   20 DO 30 I=1,15
   30 PSFITZ=PSFITZ+A(I)*B(I)
      RETURN
      END


     0SUBROUTINE TDSTRS(ENTH,PRES,TEMP,DENS,ENTRO,QUAL,DELP,DELH,TO,SO,
     1         HO,IRGN,IERR)
C     THIS CALCULATES TEMPERATURE(DEG K),DENSITY(MOLES/LITER),AND
C     ENTROPY(JOULES/MOLE DEG K) FOR GIVEN VALUES OF PRESSURE(ATM) AND
C     ENTHALPY(JOULES/MOLE). IF THE POINT FALLS IN THE TWO PHASE REGION
C     QUALITY IS ALSO DEFINED. DELP AND DELH ARE THE ALLOWABLE DESCREP-
```

```
C     ANCIES IN PRESSURE AND ENTHALPY. TO,SO,HO ARE THE REFERENCE VALUES
C     OF TEMPERATURE,ENTROPY,AND ENTHALPY ON THE IDEAL GAS SURFACE AT
C     1 ATM PRESSURE. IRGN AND IERR ARE OUTPUT FIXED POINT VARIABLES
C     INDICATING THE REGION(IRGN=1 FOR TWO PHASE REGION,IRGN=2 FOR
C     GASEOUS REGION, AND IRGN=3 FOR LIQUID REGION I.E. T LESS THAN
C     CRITICAL AND P GREATER THAN CORRESPONDING VAPOR PRESSURE) AND
C     ERRORS ENCOUNTERED DURING EXECUTION(IERR= 0 FOR PRES GREATER THAN
C     300 ATM,IERR=1 FOR PRES LESS THAN 1 ATM,IERR=2 FOR DELH/ENTH
C     LESS THAN 1.0E-08,IERR=3 FOR DELP/PRES LESS THAN 1.0E-08,(IN
C     SINGLE PRECISION THE LATTER TWO CASES MAY NOT BE SATISFIED),IERR=4
C     ,5 FOR ENTH ABOVE AND BELOW VALID RANGE RESPECTIVELY,  IERR=6 FOR
C     ITERATION NOT SATISFIED,IERR=9 FOR NORMAL OPERATION .
      DIMENSION A(15),AA(17)
      R=0.0820797
      AA(1)=R
      AA(2)=0.36684115E-01
      AA(3)=-0.10091340E+01
      AA(4)=-0.59581958E+02
      AA(5)=-0.39091633E+04
      AA(6)=0.12405065E+08
      AA(7)=0.87258515E-03
      AA(8)=-0.11885929E-01
      AA(9)=0.29165708E-05
      AA(10)=0.12473562E+04
      AA(11)=-0.61007363E+05
      AA(12)=-0.46185178E+07
      AA(13)=-0.10379526E+01
      AA(14)=0.66183734E+03
      AA(15)=-0.22051320E+05
      AA(16)=0.73071820E-06
      AA(17)=0.37656816E-02
      A16=AA(17)
      IERR=9
      CALL ARCOE(AA,A)
      H=ENTH
      P=PRES
      TUP=300.0
      TEMP=0.0
      DENS=0.0
      ENTRO=0.0
      QUAL=0.0
      IRGN=0
      PC=50.14
      C1=101.3278
      PUP=300.0
      PLO=1.0
      TLO=85.0
      TC=154.77
      DC=0.43*1000.028/32.0
      TT=54.352
      IF(P-PUP)1,1,2
    2 IERR=0
      RETURN
    1 IF(P-PLO)4,3,3
```

```
    4 IERR=1
      RETURN
    3 IF(DELH/H-1.0E-08)5,5,6
    5 IERR=2
      RETURN
    6 IF(DELP/P-1.0E-08)7,7,8
    7 IERR=3
      RETURN
    8 CONTINUE
C     CALCULATE UPPER LIMITS AND SATURATION VALUES
      DTRI=PUP/(R*TUP)
      D1=FINDPS(TUP,P   ,DTRI,A16,A)
      H1=DELH1S(P,D1,TUP,AA)+CPOHJ(TUP,TO)+HO
      IF(H-H1)11,11,10
   10 IERR=4
      RETURN
   11 IF(P-PC)9,17,17
    9 TSAT=FINDT(P,TT,TC)
      TCHEAT=TSAT-1.0
      RHOTRI=DSVGUR(TCHEAT/TC)*DC
      DSATV=FINDPS(TSAT,P,RHOTRI,A16,A)
      RHOTRI=DSATLI(TCHEAT)
      DSATL=FINDPS(TSAT,P,RHOTRI,A16,A)
      HSATV=DELH1S(P,DSATV,TSAT,AA)+CPOHJ(TSAT,TO)+HO
      HSATL=HSATV-(1.0/DSATV-1.0/DSATL)*DPDTVP(TSAT)*TSAT*101.3278
      CALL LIQCOR(SS,HSATL,TSAT)
      IF(H-HSATV)13,12,12
   12 TTRI=TSAT
      DTRI=DSATV
      GO TO 501
   13 IF(H-HSATL)15,14,14
C     CALCULATION FOR TWO PHASE REGION
   14 QUAL=(H-HSATL)/(HSATV-HSATL)
      SSATV=DELS1S(DSATV,TSAT,AA)+CPOSJ(TSAT,TO)+SO
      SSATL=SSATV-(HSATV-HSATL)/TSAT
      ENTRO=QUAL*SSATV+(1.0-QUAL)*SSATL
      DENS=QUAL*DSATV+(1.0-QUAL)*DSATL
      TEMP=TSAT
      IRGN=1
      RETURN
C     CALCULATE LOWER LIMITS
   15 H3=HSATL
      D3=DSATL
      T3=TSAT
   19 TCHEAT=TLO-1.0
       RHOTRI=DSATLI(TCHEAT)
      D2=FINDPS(TLO,P,RHOTRI,A16,A)
      PSATLO=VPN(TLO)
      DSATLL=FINDPS(TLO,PSATLO,RHOTRI,A16,A)
      RHOTRI=DSVGUR(TCHEAT/TC)*DC
      DSATVL=FINDPS(TLO,PSATLO,RHOTRI,A16,A)
     0H2=DELH1S(PSATLO,DSATVL,TLO,AA)+CPOHJ(TLO,TO)+HO -(1.0/DSATVL-1.0/
     1  DSATLL)*DPDTVP(TLO)*TLO*C1+DELHTS(P,D2,PSATLO,DSATLL,TLO,AA)
      CALL LIQCOR(SS,H2,TLO)
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```
      TTRI=TLO
      DTRI=D2
      IF(H-H2)16,701,701
   16 IERR=5
      RETURN
   17 CONTINUE
      T3=TC
      DTRI=DC*2.0
      D3=FINDPS(TC,P,DTRI,A16,A)
      H3=DELH1S(P,D3,TC,AA)+CPOHJ(TC,TO)+HO
      IF(H-H3)19,19,18
   18 CONTINUE
      DTRI=D3
      TTRI=TC
      GO TO 501
C     THIS IS THE ITERATION FOR THE GASEOUS REGION
  501 CONTINUE
      IRGN=2
      DO 550 I=1,20
      PITT=PSFITZ(TTRI,DTRI,A16,A,0)
      AX=DPDTTS(TTRI,DTRI,A16,A,0)
      BX=DPDDRS(TTRI,DTRI,A16,A,0)
      AY=DHDTRS(DTRI,TTRI,AA)
      BY=DHDDRS(DTRI,TTRI,AA)
      CX=P-PSFITZ(TTRI,DTRI,A16,A,0)
      CY=H-(DELH1S(PITT,DTRI,TTRI,AA)+CPOHJ(TTRI,TO)+HO)
      DET=AX*BY-AY*BX
      DETX=CX*BY-BX*CY
      DETY=AX*CY-CX*AY
      DT=DETX/DET
      DD=DETY/DET
      DTRI=DTRI+DD
      TTRI=TTRI+DT
      IF(ABSF(CX)-DELP)25,25,27
   25 IF(ABSF(CY)-DELH)601,601,27
   27 IF(ABSF(DT/TTRI)-1.0E-06)29 ,29 ,550
   29 IF(ABSF(DD/DTRI)-1.0E-06)601,601,550
  550 CONTINUE
      IERR=6
  601 TEMP=TTRI
      DENS=DTRI
      ENTRO=DELS1S(DENS,TEMP,AA)+CPOSJ(TEMP,TO)+SO
      IRGN=2
      RETURN
C     NEXT IS THE ITERATION FOR THE LIQUID REGION
  701 CONTINUE
      HITT=H2
      PITT=P
      DO 750 I=1,20
      BY=DHDDRS(DTRI,TTRI,AA)
      DHDTLN=((H3-H2)-BY*(D3-D2))/(T3-TLO)
      AX=DPDTTS(TTRI,DTRI,A16,A,0)
      BX=DPDDRS(TTRI,DTRI,A16,A,0)
      AY=DHDTLN
```

```
      CX=P-PITT
      CY=H-HITT
      DET=AX*BY-AY*BX
      DETX=CX*BY-BX*CY
      DETY=AX*CY-CX*AY
      DT=DETX/DET
      DD=DETY/DET
      DTRI=DTRI+DD
      TTRI=TTRI+DT
      PS=VPN(TTRI)
C     A TEMPERATURE SLIGHTLY BELOW TTRI IS USED HERE TO IMPROVE THE
C     CHANCE OF SUCCESS NEAR CRITICAL TEMPERATURE
      TCHEAT=(TTRI-1.0)
      DVTRI=DSVGUR(TCHEAT/TC)*DC
      DSATVT=FINDPS(TTRI,PS,DVTRI,A16,A)
      DLTRI=DSATLI(TCHEAT)
      DSATLT=FINDPS(TTRI,PS,DLTRI,A16,A)
      PITT=PSFITZ(TTRI,DTRI,A16,A,0)
     0HITT=DELH1S(PS,DSATVT,TTRI,AA)+CPOHJ(TTRI,TO)+HO-(1.0/DSATVT-
     1  1.0/DSATLT)*DPDTVP(TTRI)*TTRI*C1+DELHTS(PITT,DTRI,PS,DSATLT,
     2    TTRI,AA)
       CALL LIQCOR(SS,HITT,TTRI)
      IF(H-HITT)711,711,721
  711 H3=HITT
      T3=TTRI
      D3=DTRI
      GO TO 731
  721 D2=DTRI
      H2=HITT
      TLO=TTRI
  731 CONTINUE
      IF(ABSF(H-HITT)-DELH)733,733,735
  733 IF(ABSF(P-PITT)-DELP)761,761,735
  735 IF(ABSF(DD/DTRI)-1.0E-06)737,737,750
  737 IF(ABSF(DT/TTRI)-1.0E-06)761,761,750
  750 CONTINUE
      IERR=6
  761 TEMP=TTRI
      DENS=DTRI
     0ENTRO=DELS1S(DSATVT,TEMP,AA)+CPOSJ(TEMP,TO)+SO-(1./DSATVT-1./
     1  DSATLT)*DPDTVP(TEMP)*C1+DELSTS(DENS,DSATLT,TEMP,AA)
      CALL LIQCOR(ENTRO,HH,TEMP)
      IRGN=3
      RETURN
      END


      SUBROUTINE THSTRS(P,D,T,H,S,Q,DP,TO,SO,HO,IRGN,IERR)
C     THIS CALCULATES TENPERATURE(DEG K),ENTHALPY(JOULES/MOLE) AND
C     ENTROPY(JOULES/MOLE DEG K) FOR GIVEN VALUES OF PRESSURE(ATM) AND
C     DENSITY(MOLES/LITER). IF THE POINT FALLS IN THE TWO PHASE REGION
C     QUALITY(Q) IS ALSO DEFINED. DP IS THE ALLOWABLE DESCREPANCY IN
C     PRESSURE. TO,SO,HO ARE THE REFERENCE VALUES OF TEMPERATURE,ENTROPY
```

```
C     AND ENTHALPY ON THE IDEAL GAS SURFACE AT 1 ATM PRESSURE. IRGN AND
C     IERR ARE OUTPUT FIXED POINT VARIABLES INDICATING THE REGION(IRGN=1
C     FOR TWO PHASE REGION,IRGN=2 FOR GASEOUS REGION, AND IRGN=3 FOR
C     LIQUID REGION I.E. T LESS THAN CRITICAL AND P GREATER THAN THE
C     CORRESPONDING VAPOR PRESSURE) AND ERRORS ENCOUNTERED DURING
C     EXECUTION(IERR=0 FOR PRESSURE GREATER THAN 300 ATM,IERR=1 FOR
C     LESS THAN 1 ATM,IERR=2 FOR DP/P LESS THAN 1.0E-08,IERR=4 AND 5
C     FOR TEMPERATURE ABOVE AND BELOW VALID RANGE RESPECTIVELY, IERR=6 FOR
C     ITERATION NOT SATISFIED, AND IERR=9 FOR NORMAL OPERATION.
      DIMENSION A(15),AA(17)
      R=0.0820797
      AA(1)=R
      AA(2)=0.36684115E-01
      AA(3)=-0.10091340E+01
      AA(4)=-0.59581958E+02
      AA(5)=-0.39091633E+04
      AA(6)=0.12405065E+08
      AA(7)=0.87258515E-03
      AA(8)=-0.11885929E-01
      AA(9)=0.29165708E-05
      AA(10)=0.12473562E+04
      AA(11)=-0.61007363E+05
      AA(12)=-0.46185178E+07
      AA(13)=-0.10379526E+01
      AA(14)=0.66183734E+03
      AA(15)=-0.22051320E+05
      AA(16)=0.73071820E-06
      AA(17)=0.37656816E-02
      A16=AA(17)
      IERR=9
      CALL ARCOE(AA,A)
      TUP=300.0
      T=0.0
      S=0.0
      Q=0.0
      IRGN=0
      PC=50.14
      C1=101.3278
      PUP=300.0
      PLO=1.0
      TLO=85.0
      H=0.0
      TC=154.77
      TT=54.353
      DC=0.43*1000.028/32.0
      IF(P-PUP)1,1,2
    2 IERR=0
      RETURN
    1 IF(P-PLO)4,3,3
    4 IERR=1
      RETURN
    3 IF(DP/P-1.0E-08)5,5,8
    5 IERR=2
      RETURN
```

```
    8 CONTINUE
      IF(P-PC)10,15,15
C     CALCULATE SATURATION TEMPERATURE AND DENSITIES
   10 TSAT=FINDT(P,TT,TC)
      TCHEAT=TSAT-1.0
      DVTRI=DSVGUR(TCHEAT/TC)*DC
      DLTRI=DSATLI(TCHEAT)
      DSATV=FINDPS(TSAT,P,DVTRI,A16,A)
      DSATL=FINDPS(TSAT,P,DLTRI,A16,A)
      IF(D-DSATV)13,13,11
   13 CONTINUE
      TTRI=(3.0/8.0)*(P/PC+3.0*(D/DC)**2)*(DC/D-1.0/3.0)*TC
      T=FINTPS(D,P,TTRI,A16,A)
      IF(T-1.E-08)24,24,25
   24 IERR=6
      RETURN
   25 GO TO 70
   11 IF(D-DSATL)14,14,15
C     CALCULATION FOR TWO PHASE REGION
   14 Q=(D-DSATL)/(DSATV-DSATL)
      SSATV=DELS1S(DSATV,TSAT,AA)+CPOSJ(TSAT,TO)+SO
      SCROS=(1.0/DSATV-1.0/DSATL)*DPDTVP(TSAT)*C1
      HCROS=SCROS*TSAT
      SSATL=SSATV-SCROS
      HSATV=DELH1S(P,DSATV,TSAT,AA)+CPOHJ(TSAT,TO)+HO
      HSATL=HSATV-HCROS
      T=TSAT
      CALL LIQCOR(SSATL,HSATL,TSAT)
      S=Q*SSATV+(1.0-Q)*SSATL
      H=Q*HSATV+(1.0-Q)*HSATL
      IRGN=1
      RETURN
   15 CONTINUE
      TTRI=(3.0/8.0)*(P/PC+3.0*(D/DC)**2)*(DC/D-1.0/3.0)*TC
      IF(TTRI-TLO)17,18,18
   17 TTRI=TLO
   18 CONTINUE
      T=FINTPS(D,P,TTRI,A16,A)
      IF(T-1.E-08)54,54,55
   54 IERR=6
      RETURN
   55 IF(T-TC)170,70,70
   70 CONTINUE
      IRGN=2
      IF(T-TUP)80,80,71
   71 IERR=4
      RETURN
   80 H=DELH1S(P,D,T,AA)+CPOHJ(T,TO)+HO
      S=DELS1S(D,T,AA)+CPOSJ(T,TO)+SO
      RETURN
  170 CONTINUE
      IF(T-TLO)171,180,180
  171 IERR=5
      RETURN
```

```
  180 CONTINUE
      IRGN=3
      PS=VPN(T)
      TCHEAT=T-1.0
      DVTRI=DSVGUR(TCHEAT/TC)*DC
      DLTRI=DSATLI(TCHEAT)
      DSATV=FINDPS(T,PS,DVTRI,A16,A)
      DSATL=FINDPS(T,PS,DLTRI,A16,A)
      SCROS=(1.0/DSATV-1.0/DSATL)*DPDTVP(T)*C1
      HCROS=SCROS*T
     0H=DELH1S(PS,DSATV,T,AA)+CPOHJ(T,TO)+HO-HCROS+DELHTS(P,D,PS,DSATL,
     1     T,AA)
      S=DELS1S(DSATV,T,AA)+CPOSJ(T,TO)+SO-SCROS+DELSTS(D,DSATL,T,AA)
      CALL LIQCOR(S,H,T)
      RETURN
      END


      FUNCTION VPN(TEMP)
C     VAPOR PRESSURE OF OXYGEN ACCORDING TO THE EQUATION IN NBS REPORT
C     7922. TEMPERATURE IN DEG K AND VPN IN ATM.
      T=TEMP
      A=0.13750055E-03
      B=-0.54998814E-01
      C=0.17023470E+01
      D=0.66564191E+01
      E=-0.94512173E+03
      P=EXPF(D+E/T+B*T+C*LOGF(T)+A*T*T)
      VPN=P
      RETURN
      END
```

APPENDIX B

Sample calculations of thermodynamic properties with pressure-enthalpy and pressure-density as input coordinates are presented. Comparisons with the values listed by Stewart, et al. [1963] are included to illustrate the consistency of these calculations. Although the speed of computation is dependent upon the values of the coordinates, a speed of 115 points per minute (randomly distributed) has been obtained.

```
*       ID(3150420,JHPHPD,HUSTJG,1,0,3)     386
*       XEQ
*       LABEL
CJHPHPD
        DIMENSION FMT(12),IDENT(12)
  100   FORMAT(12A6/12A6)
        READ INPUT TAPE 5,100,IDENT,FMT
        READ INPUT TAPE 5,FMT,TC,PC,DC,PT,TT,TO,SO,HO
        WRITE OUTPUT TAPE 6,100,IDENT,FMT
        WRITE OUTPUT TAPE 6,FMT,TC,PC,DC,PT,TT,TO,SO,HO
        READ INPUT TAPE 5,100,IDENT,FMT
        WRITE OUTPUT TAPE 6,400
  400   FORMAT(1H1)
        WRITE OUTPUT TAPE 6,500
        WRITE OUTPUT TAPE 6,300
  500   FORMAT(95H   PRESSURE      TEMPERATURE      DENSITY         ENTROPY
       1   ENTHALPY        QUALITY  REGION ERROR  )
   10   READ INPUT TAPE 5,FMT,P,T,D,S,H,QIN,IREGN,IERIN
        DD=D*1000.028/32.0
        SS=S*32.0
        HH=H*32.0
       0CALL TDSTRS(HH,P,TCALHP,DCALHP,SCALHP,QHP, 0.00001*P, 0.00001*HH,
       1       TO,SO,HO,IRGNHP,IERHP)
       0CALL THSTRS(P,DD,TCALPD,HCALPD,SCALPD,QPD, 0.00001*P,TO,SO,HO,
       1      IRGNPD,IERPD)
  200   FORMAT(6E14.6,2I4,33H  INPUT DATA FROM NBS REPORT 7922,/,6E14.6,
       1  2I4,39H  CALCULATED FROM PRESSURE AND ENTHALPY,/,6E14.6,2I4,
       2     39H  CALCULATED FROM PRESSURE AND DENSITY    )
       0WRITE OUTPUT TAPE 6,200,P,T,DD,SS,HH,QIN,IREGN,IERIN,
       1     P,TCALHP,DCALHP,SCALHP,HH,QHP,IRGNHP,IERHP,
       2 P,TCALPD,DD,SCALPD,HCALPD,QPD,IRGNPD,IERPD,
        WRITE OUTPUT TAPE 6,300
  300   FORMAT(1H0)
        GO TO 10
        END
*       DATA
CRITICAL DATA FOR OXYGEN(CRIT. PT.,TRIPLE PT.,TO,SO,HO)
(E16.8)
    .15478    E+03
    .5014     E+02
    .13437876E+02
    .14473684E-02
    .54352    E+02
   0.9        E+02
   0.17021230E+03
    .11405399E+05
P,T,D,S,H,Q,IREGN,IERIN(ATM,DEG K,G/CC,JOULE/G)FROM NBS REPORT 7922
(F8.2,F9.3,E12.5,F9.4,F8.2,F6.2,2I2)
    50.0    154.707   .32389E+00    4.3415   328.94    .99 1 9
     1.5     90.0     .11408E+01    2.9328   140.48        3 9
```

40.0	148.982	.68834E+00	3.9239	263.15	.01	1	9
60.0	90.0	.11536E+01	2.9106	143.65		3	9
50.0	154.0	.60328E+00	4.0320	281.08		3	9
50.0	155.0	.29779E+00	4.3795	334.82		2	9
1.0	90.0	.11406E+01	2.9330	140.46		3	9
1.0	91.0	.44217E-02	5.3154	355.35		2	9
1.0	300.0	.13003E-02	6.4151	547.57		2	9
300.0	300.0	.38922E-00	4.7723	492.32		2	9

COMPUTER OUTPUT FROM PROGRAM JHPHPD (Sample Calculations of Oxygen Thermodynamic Properties).

PRESSURE	TEMPERATURE	DENSITY	ENTROPY	ENTHALPY	QUALITY	REGION	ERROR	
0.500000E 02	0.154707E 03	0.101218E 02	0.138928E 03	0.105261E 05	0.990000E 00	1	9	INPUT DATA FROM NBS REPORT 7922
0.500000E 02	0.154707E 03	0.101213E 02	0.138928E 03	0.105261E 05	0.990059E 00	1	9	CALCULATED FROM PRESSURE AND ENTHALPY
0.500000E 02	0.154707E 03	0.101218E 02	0.138927E 03	0.105260E 05	0.989983E 00	1	9	CALCULATED FROM PRESSURE AND DENSITY
0.150000E 01	0.900000E 02	0.356510E 02	0.938496E 02	0.449536E 04	-0.	3	9	INPUT DATA FROM NBS REPORT 7922
0.150000E 01	0.899986E 02	0.356499E 02	0.938478E 02	0.449536E 04	0.	3	9	CALCULATED FROM PRESSURE AND ENTHALPY
0.150000E 01	0.899918E 02	0.356510E 02	0.938436E 02	0.449498E 04	0.	3	9	CALCULATED FROM PRESSURE AND DENSITY
0.400000E 02	0.148982E 03	0.215112E 02	0.125565E 03	0.842080E 04	1.000000E-02	1	9	INPUT DATA FROM NBS REPORT 7922
0.400000E 02	0.148982E 03	0.215098E 02	0.125565E 03	0.842080E 04	0.100869E-01	1	9	CALCULATED FROM PRESSURE AND ENTHALPY
0.400000E 02	0.148982E 03	0.215112E 02	0.125564E 03	0.842054E 04	0.999471E-02	1	9	CALCULATED FROM PRESSURE AND DENSITY
0.600000E 02	0.900000E 02	0.360510E 02	0.931392E 02	0.459680E 04	-0.	3	9	INPUT DATA FROM NBS REPORT 7922
0.600000E 02	0.899969E 02	0.360511E 02	0.931377E 02	0.459680E 04	0.	3	9	CALCULATED FROM PRESSURE AND ENTHALPY
0.600000E 02	0.899976E 02	0.360510E 02	0.931381E 02	0.459682E 04	0.	3	9	CALCULATED FROM PRESSURE AND DENSITY
0.500000E 02	0.154000E 03	0.188530E 02	0.129024E 03	0.899456E 04	-0.	3	9	INPUT DATA FROM NBS REPORT 7922
0.500000E 02	0.154000E 03	0.188538E 02	0.129024E 03	0.899456E 04	0.	3	9	CALCULATED FROM PRESSURE AND ENTHALPY
0.500000E 02	0.154000E 03	0.188530E 02	0.129025E 03	0.899470E 04	0.	3	9	CALCULATED FROM PRESSURE AND DENSITY
0.500000E 02	0.155000E 03	0.930620E 01	0.140144E 03	0.107142E 05	-0.	2	9	INPUT DATA FROM NBS REPORT 7922
0.500000E 02	0.155000E 03	0.930579E 01	0.140143E 03	0.107142E 05	0.	2	9	CALCULATED FROM PRESSURE AND ENTHALPY
0.500000E 02	0.155000E 03	0.930620E 01	0.140143E 03	0.107141E 05	0.	2	9	CALCULATED FROM PRESSURE AND DENSITY
0.100000E 01	0.900000E 02	0.356447E 02	0.938560E 02	0.449472E 04	-0.	3	9	INPUT DATA FROM NBS REPORT 7922
0.100000E 01	0.900024E 02	0.356457E 02	0.938565E 02	0.449472E 04	0.	3	9	CALCULATED FROM PRESSURE AND ENTHALPY
0.100000E 01	0.900084E 02	0.356447E 02	0.938602E 02	0.449505E 04	0.	3	9	CALCULATED FROM PRESSURE AND DENSITY
0.100000E 01	0.910000E 02	0.138182E-00	0.170093E 03	0.113712E 05	-0.	2	9	INPUT DATA FROM NBS REPORT 7922
0.100000E 01	0.910024E 02	0.138177E-00	0.170093E 03	0.113712E 05	0.	2	9	CALCULATED FROM PRESSURE AND ENTHALPY
0.100000E 01	0.909991E 02	0.138182E-00	0.170092E 03	0.113711E 05	0.	2	9	CALCULATED FROM PRESSURE AND DENSITY
0.100000E 01	0.300000E 03	0.406355E-01	0.205283E 03	0.175222E 05	-0.	2	9	INPUT DATA FROM NBS REPORT 7922
0.100000E 01	0.300000E 03	0.406341E-01	0.205283E 03	0.175222E 05	0.	2	9	CALCULATED FROM PRESSURE AND ENTHALPY
0.100000E 01	0.299990E 03	0.406355E-01	0.205282E 03	0.175219E 05	0.	2	9	CALCULATED FROM PRESSURE AND DENSITY
0.300000E 03	0.300000E 03	0.121635E 02	0.152714E 03	0.157542E 05	-0.	2	9	INPUT DATA FROM NBS REPORT 7922
0.300000E 03	0.299999E 03	0.121634E 02	0.152715E 03	0.157542E 05	0.	2	9	CALCULATED FROM PRESSURE AND ENTHALPY
0.300000E 03	0.299999E 03	0.121635E 02	0.152715E 03	0.157542E 05	0.	2	9	CALCULATED FROM PRESSURE AND DENSITY